



[졸업작품전 - 작품]

Self-Supervised Discovery of Neural Circuits with Graph Neural Networks

■ 정우열 : 융합전자공학부 2019089825



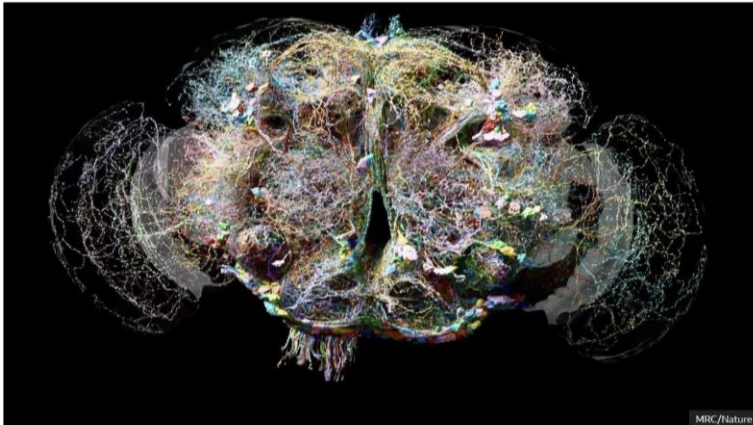
Background

Fly brain breakthrough 'huge leap' to unlock human mind

3 October 2024

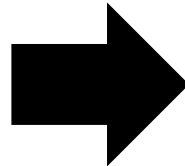
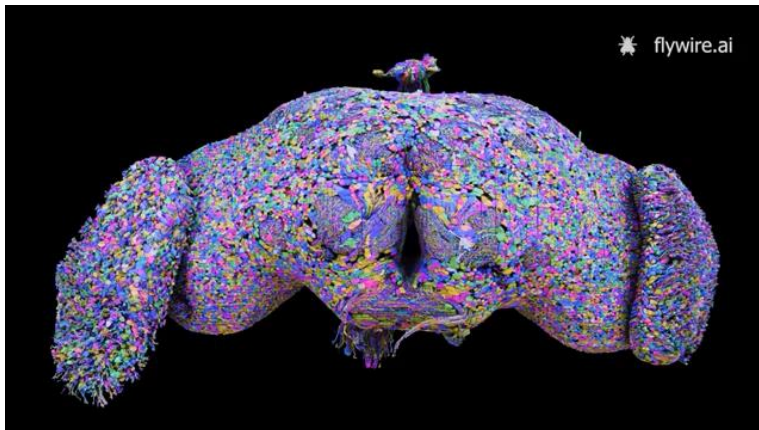
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Pallab Ghosh
Science Correspondent • @BBCPallab



As beautiful as it is complex, the fly's brain has more than 130,000 wires with 50 million intricate connections

MRC/Nature

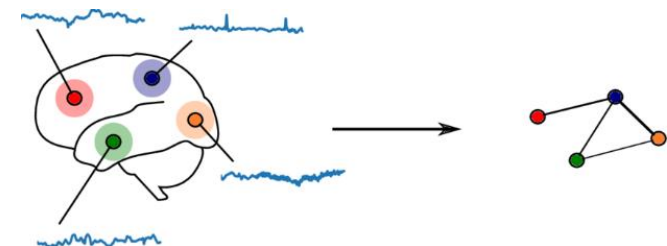


Human Connectome Project

The findings from Human Connectome Project will help transform our understanding of the human mind and brain in health, and in disease.

- Alzheimer's Disease (Decreased connectivity and Hippocampus changes)
- Anxiety (Increased connectivity and Amygdala changes)
- ADHD (Altered connectivity)
- Autism (Altered connectivity and Cerebellum, Thalamus changes)
- Cognitive Decline (Disruption of connectivity and motor networks)

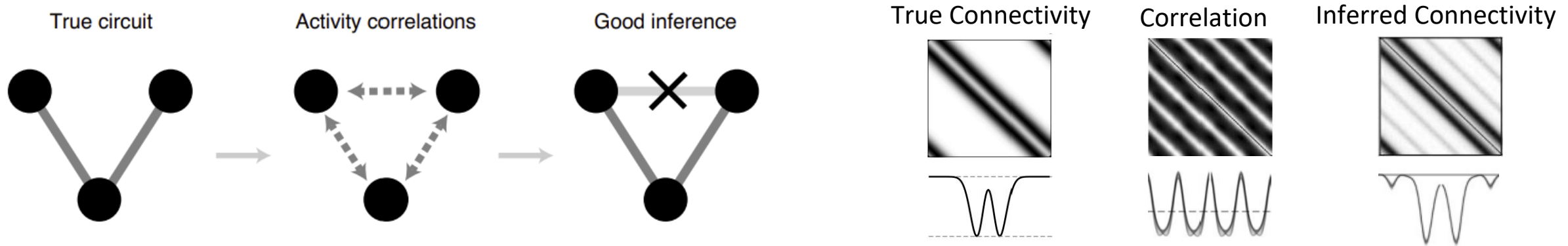
Neural Connectivity Inference



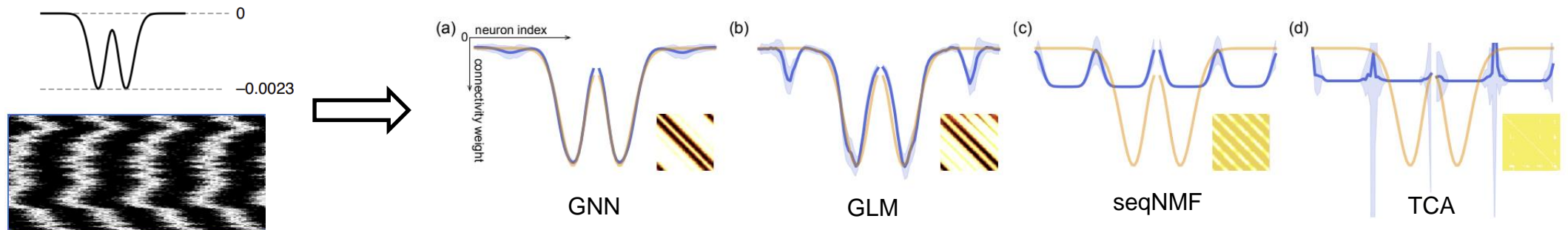
Related work

Neural Connectivity inference using GNNs

Systematic errors in connectivity inferred from activity in strongly recurrent network, Fiete, 2020



Graph Neural Networks for Connectivity Inference in Spatially Patterned Neural Responses, Park, 2022



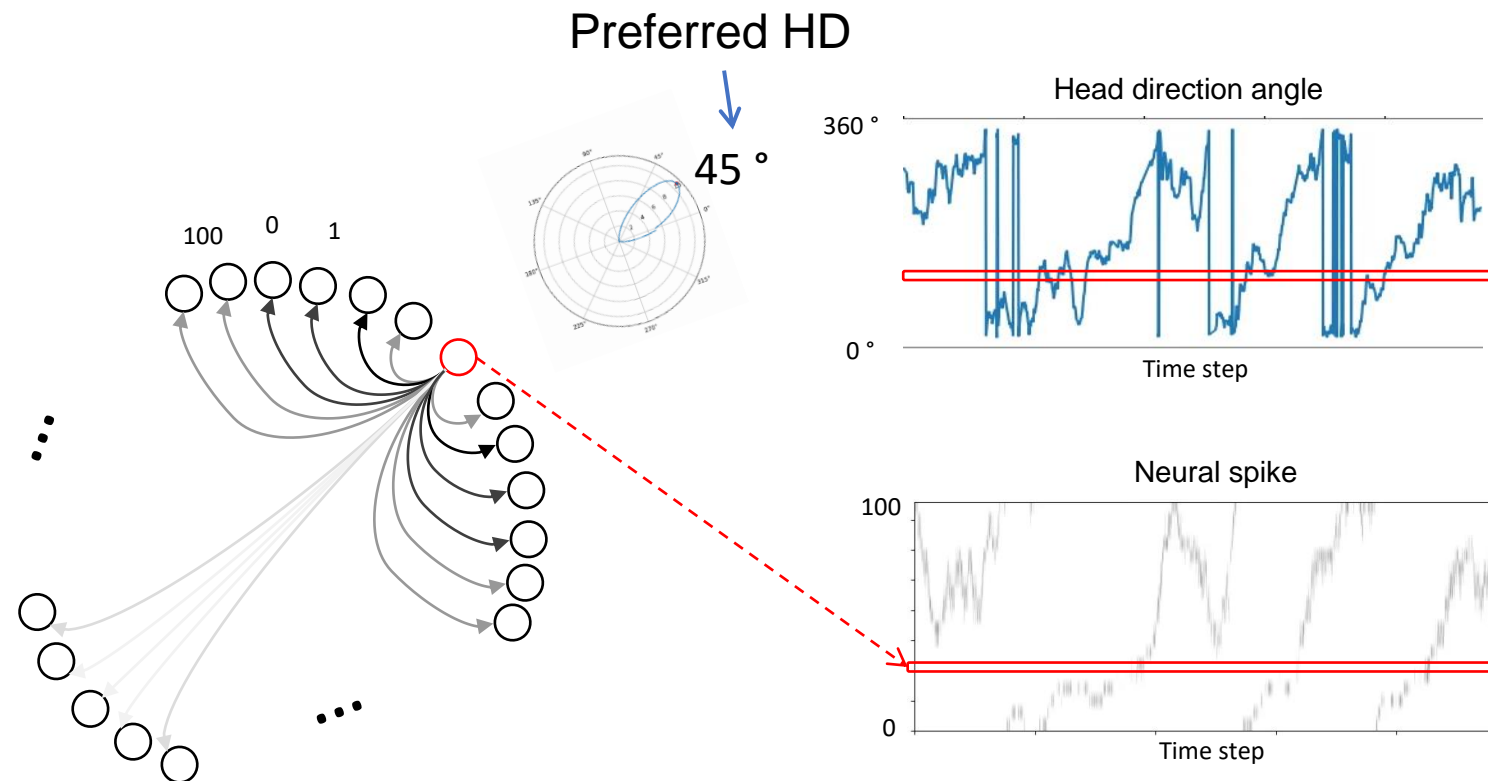
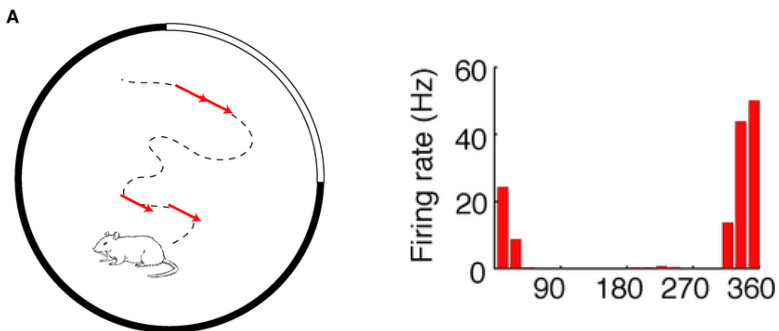
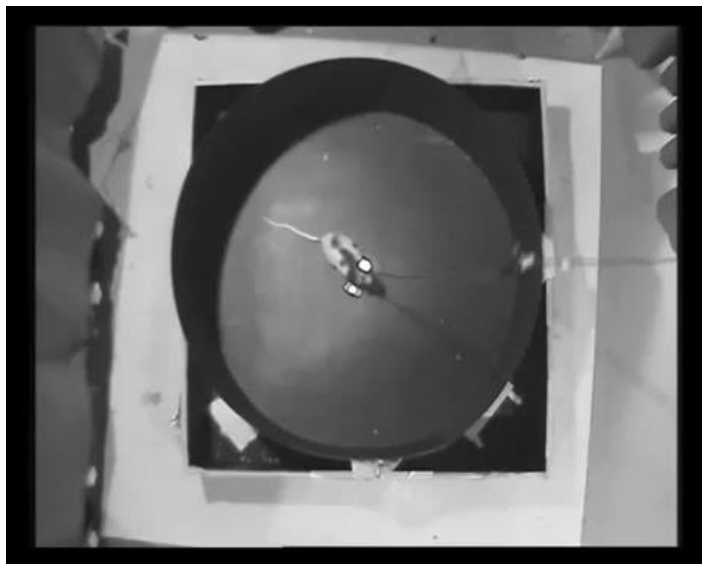
Our proposal

- Inferring Neural Connectivity of **Mouse Head Direction Cells** using GNNs
- Proposing **Hidden Neurons** to Enhance Neural Connectivity Inference and Time Series Forecasting with GNNs

Methods

Dataset

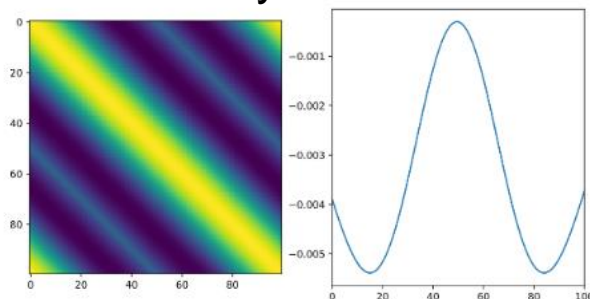
Head Direction Cell



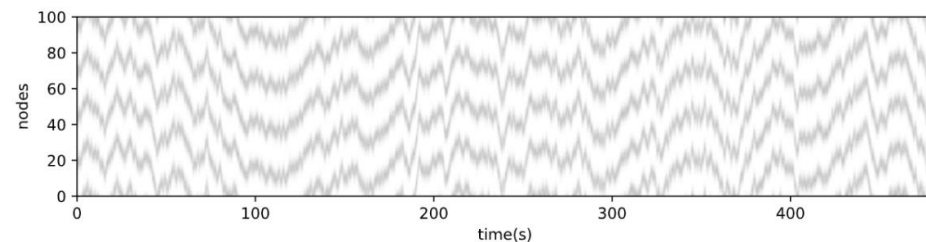
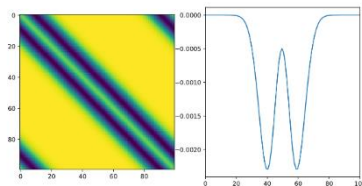
Dataset

Synthetic dataset

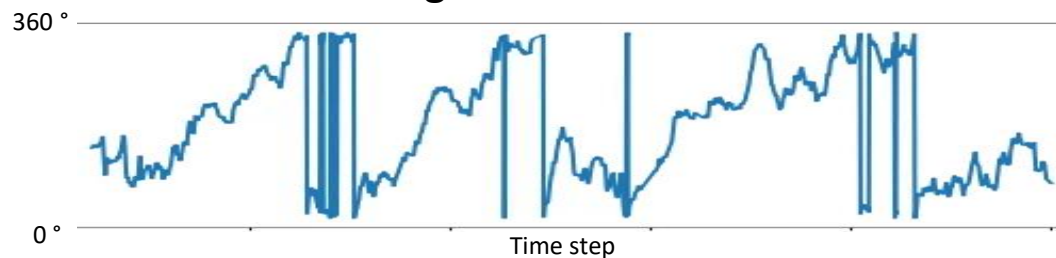
Connectivity



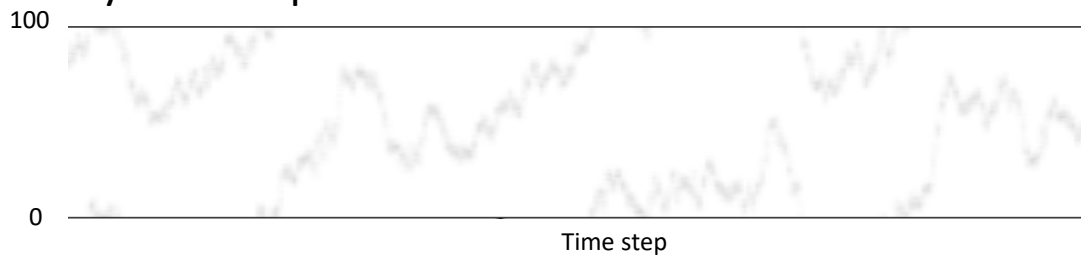
Systematic errors in connectivity inferred from activity in strongly recurrent network, Fiete, 2020



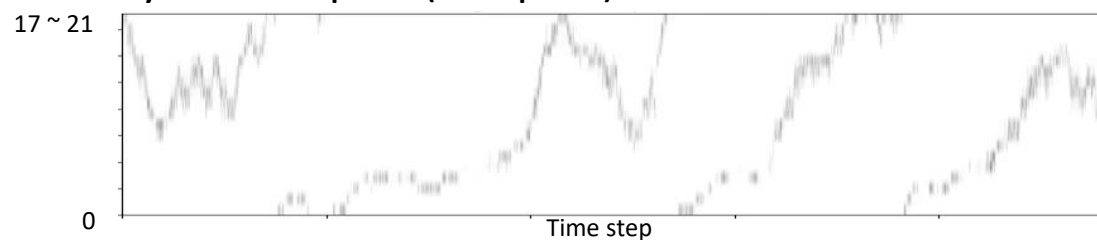
Head direction angle



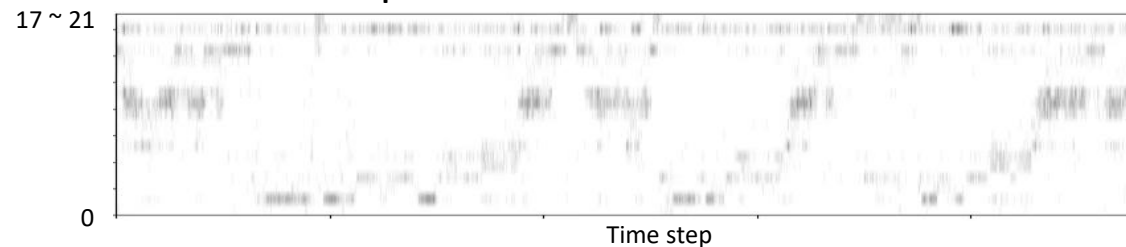
Synthetic spike



Synthetic spike (sampled)

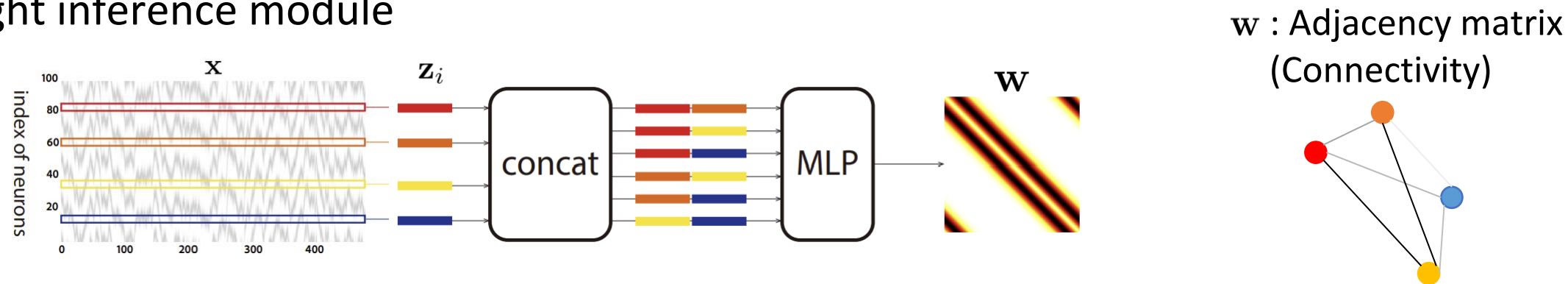


Real mouse spike

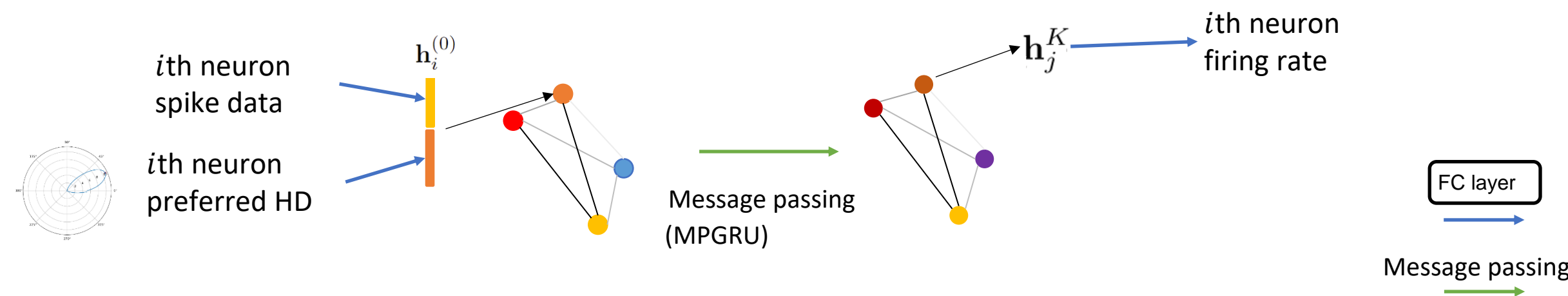


Model

Weight inference module



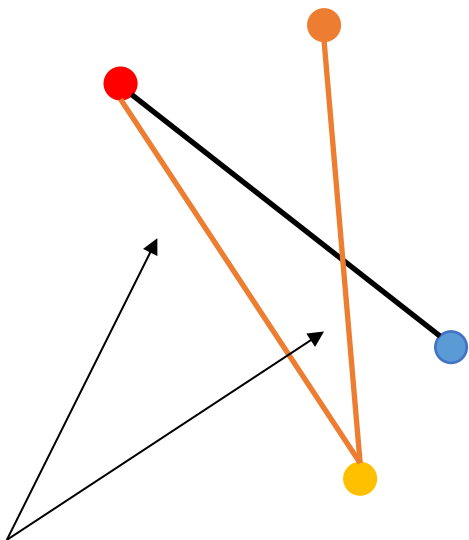
Spike prediction module



Model

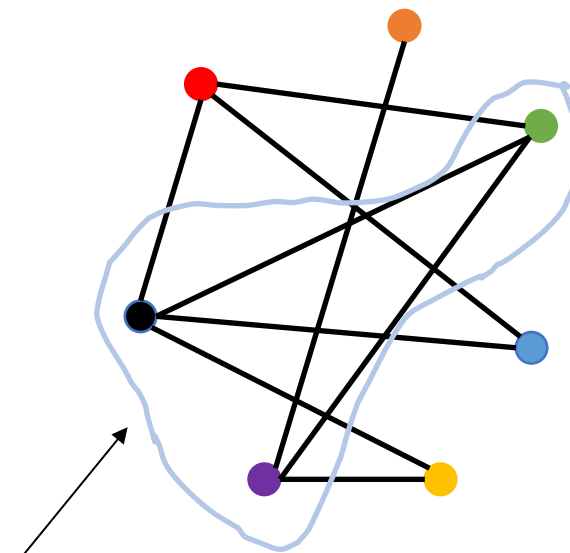
To improve spike prediction accuracy by accounting for interactions with unobserved neurons, we incorporated **Hidden neurons** into our model

Connectivity inferred from
observed neurons only



Wrong Inference

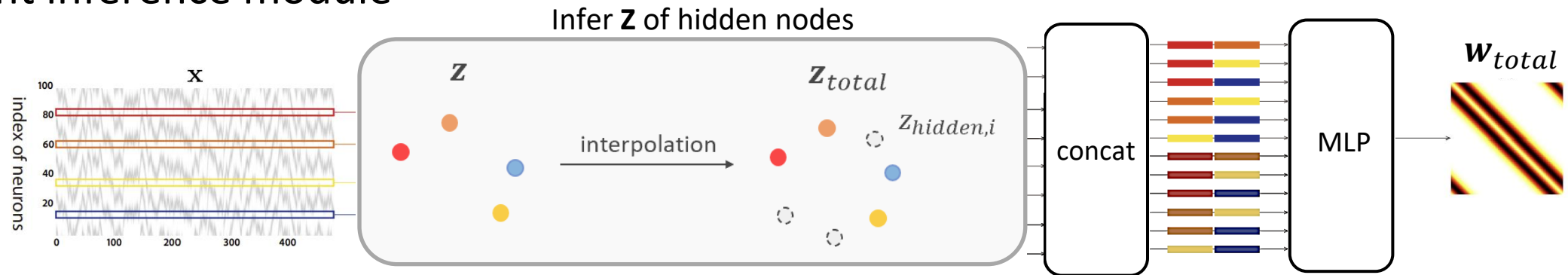
Actual connectivity among
interacting neurons



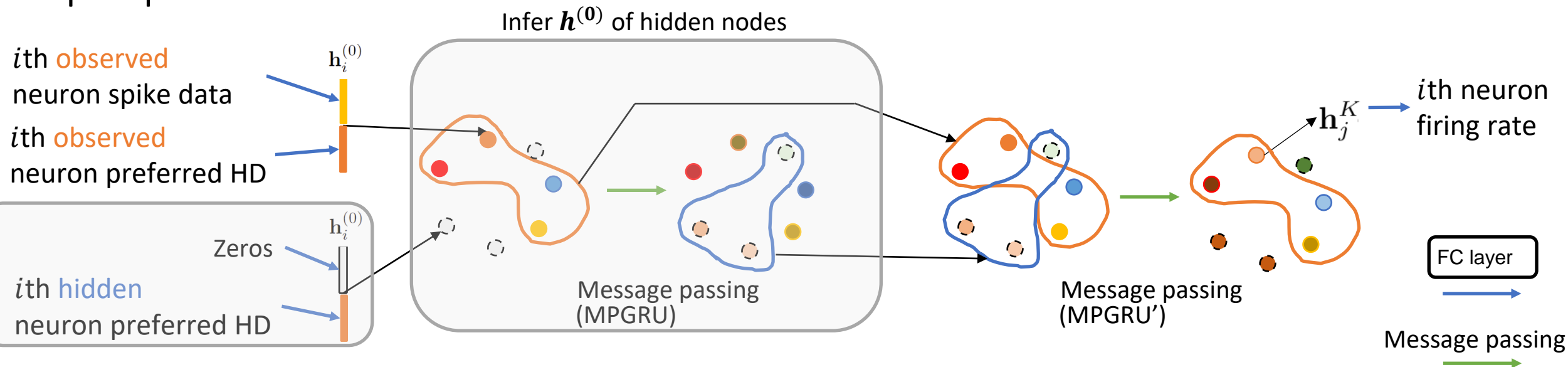
Hidden neurons

Model (with Hidden neurons)

Weight inference module



Spike prediction module

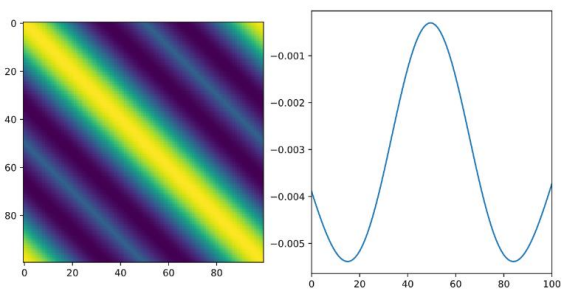
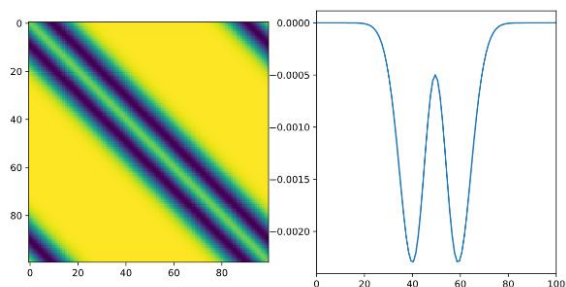


Results

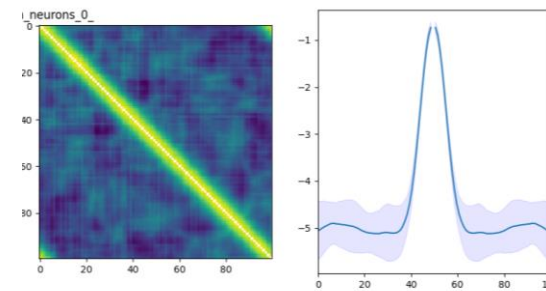
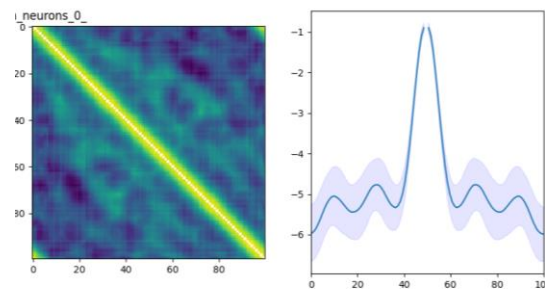
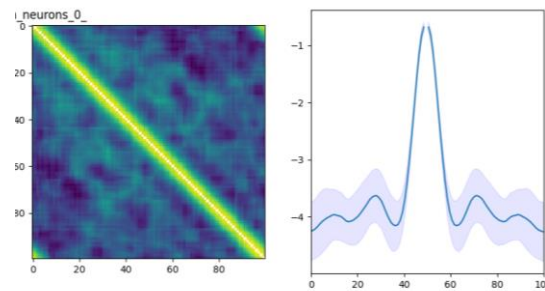
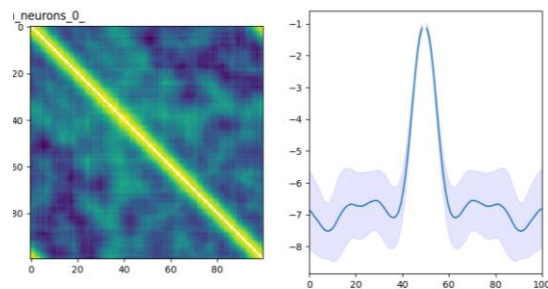
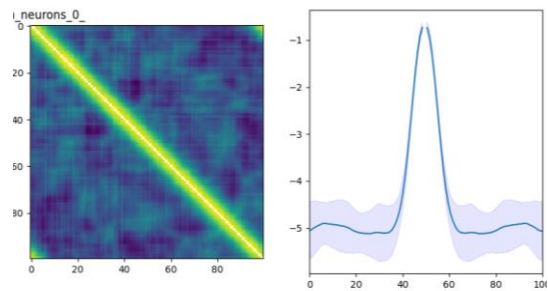
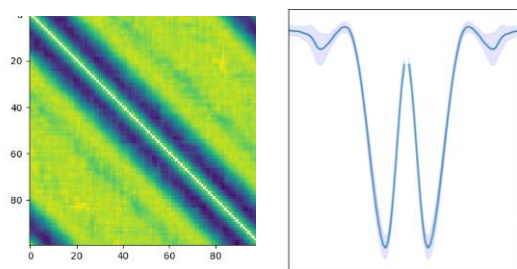
Results

Connectivity inference (Synthetic data)

True Connectivity



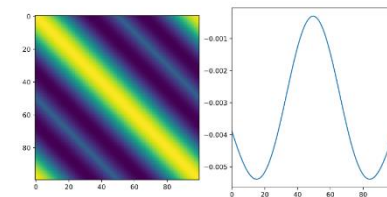
Inferred Connectivity



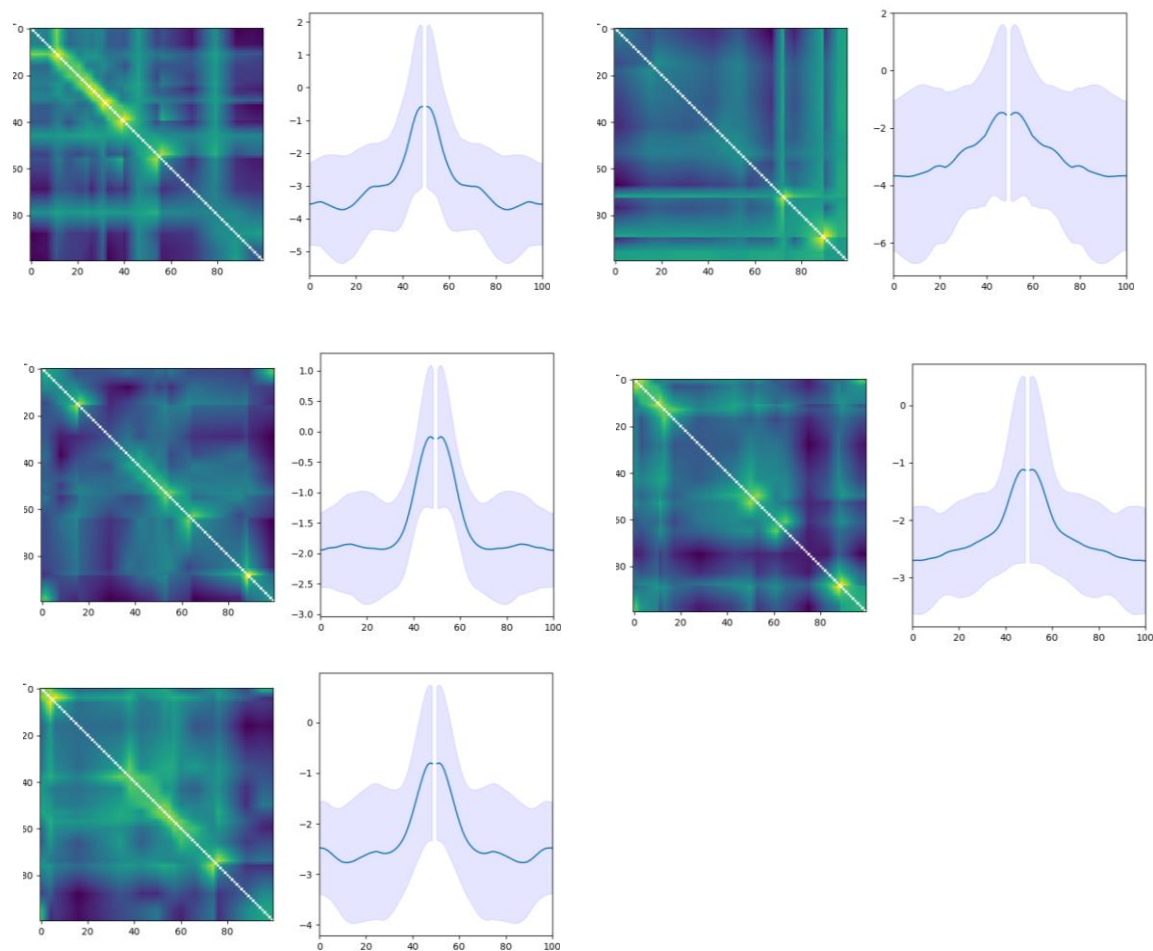
Results

Connectivity inference (Sampled synthetic data)

True Connectivity

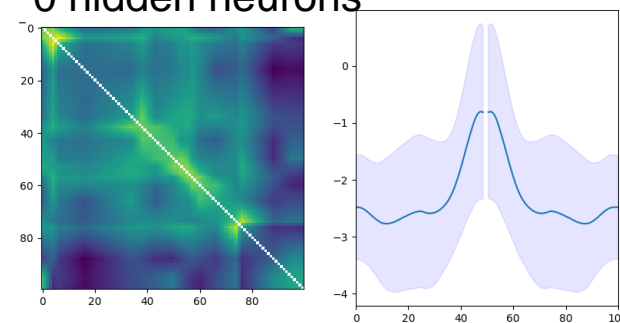


Inferred Connectivity

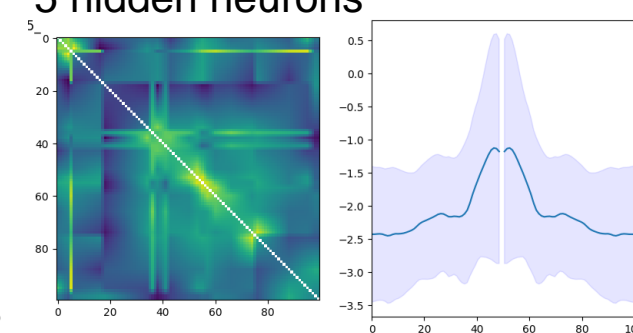


With hidden neurons

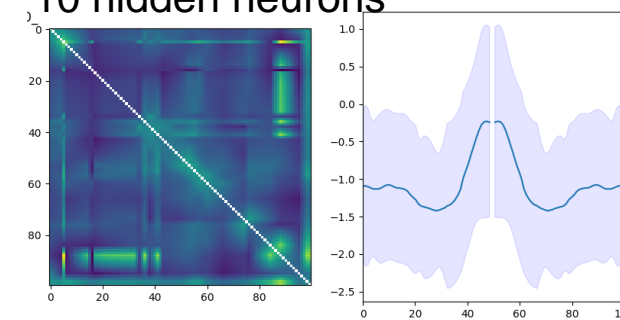
0 hidden neurons



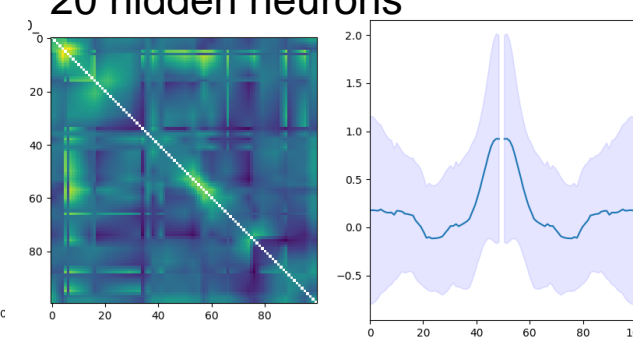
5 hidden neurons



10 hidden neurons



20 hidden neurons



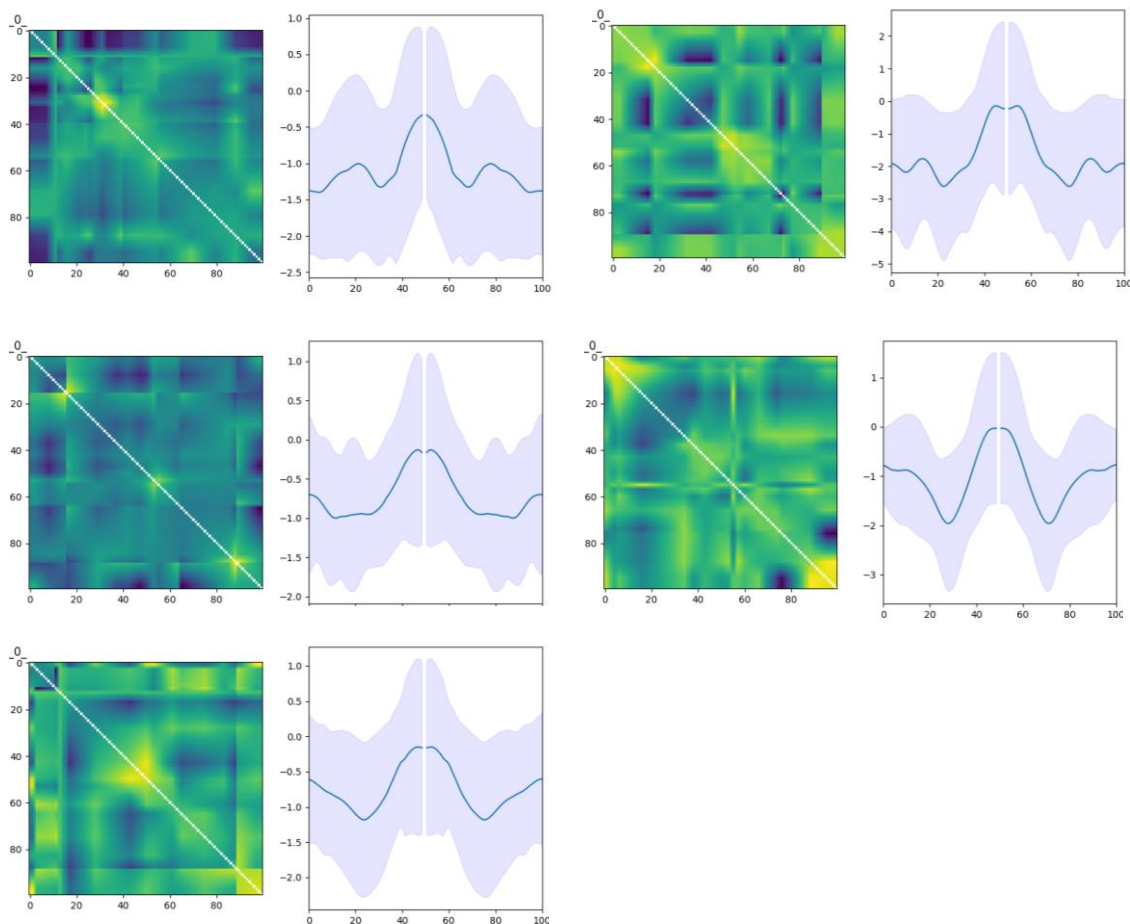
Results

Connectivity inference (Real mouse data)

True Connectivity

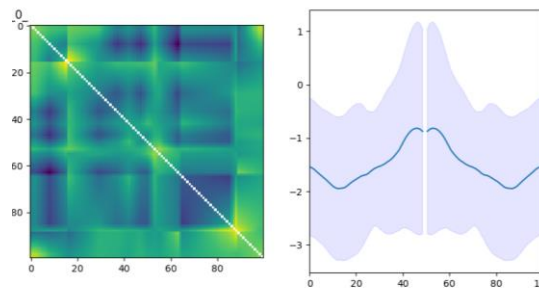
?

Inferred Connectivity

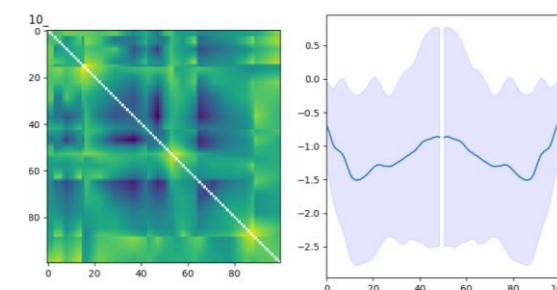


With hidden neurons

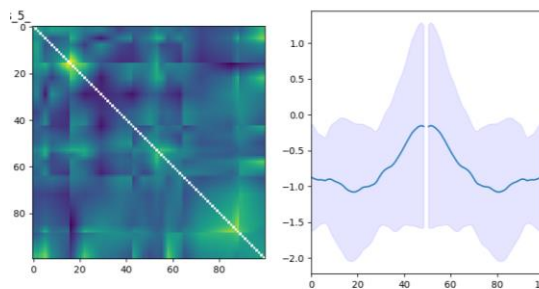
0 hidden neurons



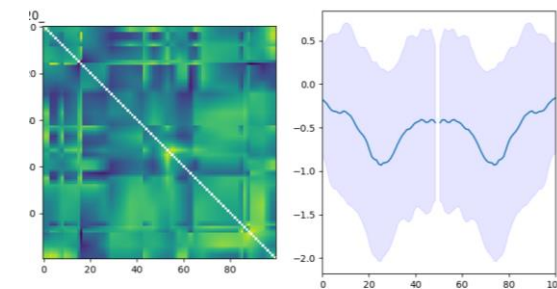
5 hidden neurons



10 hidden neurons



20 hidden neurons



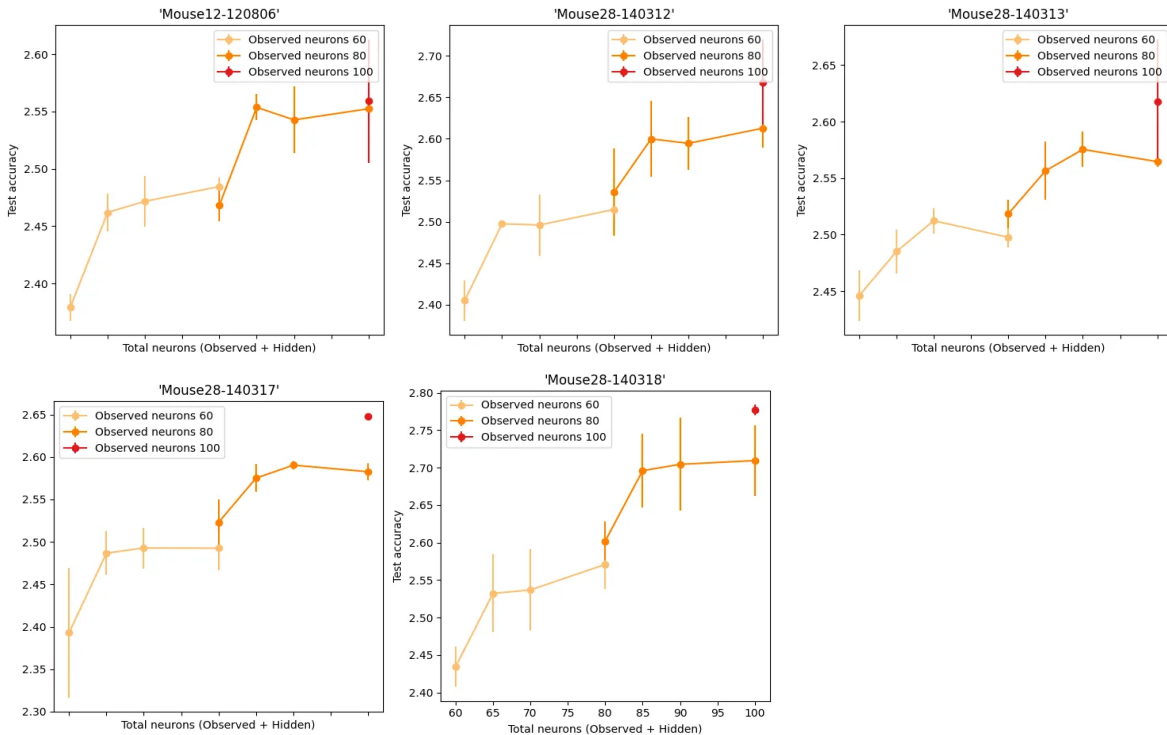
Results

Effect of hidden neurons in Test accuracy

Synthetic data

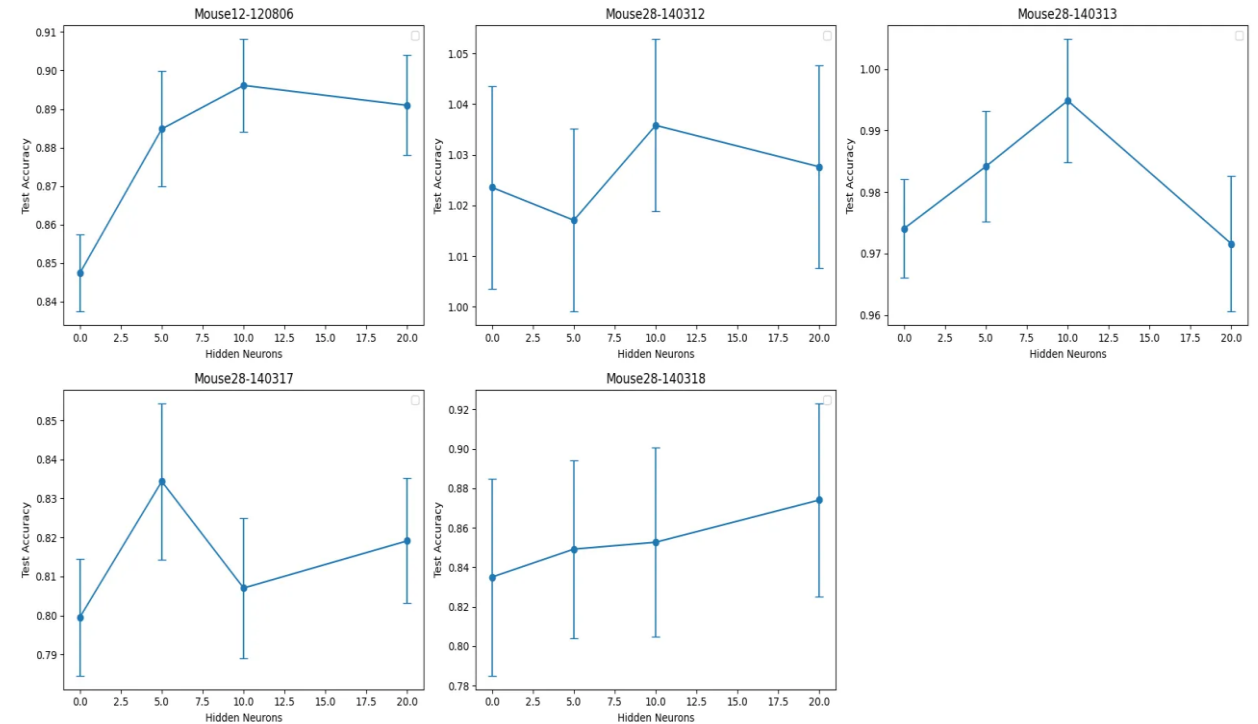
Observed neurons 60, 80, 100

Hidden neurons 0, 5, 10, 20



Real mouse data

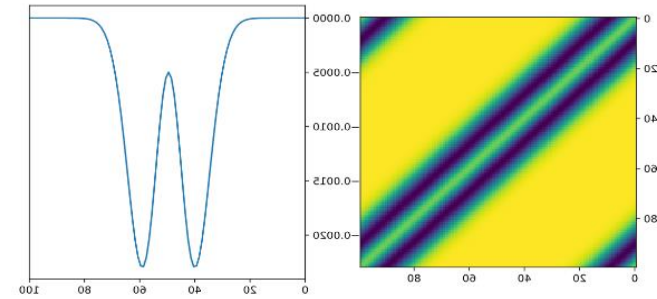
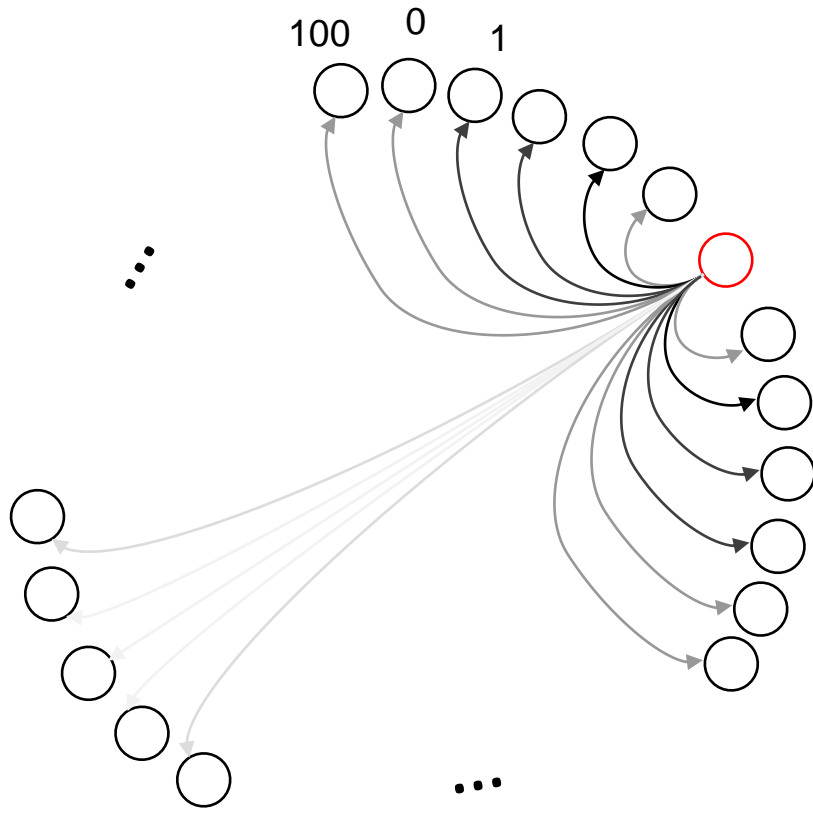
Hidden neurons 0, 5, 10, 20



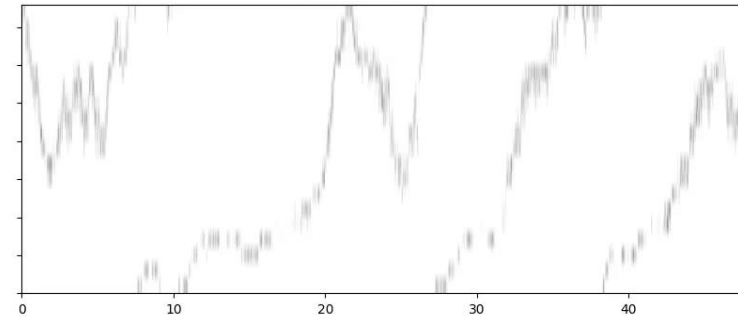
Thank you

Dataset

Synthetic dataset



$$W_{\text{mexican hat}}^{ij} = e^{-d_{ij}^2/2\sigma_1^2} - ae^{-d_{ij}^2/2\sigma_2^2}$$



$$\theta^* = \frac{2\pi}{100} \mathbf{i}$$

$$b = \alpha(1 + \beta \hat{e}_\theta \cdot \hat{e}_{\theta^*})$$

$$I_t = \gamma s_t W + b(1 + \xi)$$

$$\xi = \sigma_\xi(n_\xi > \text{threshold}_\xi)$$

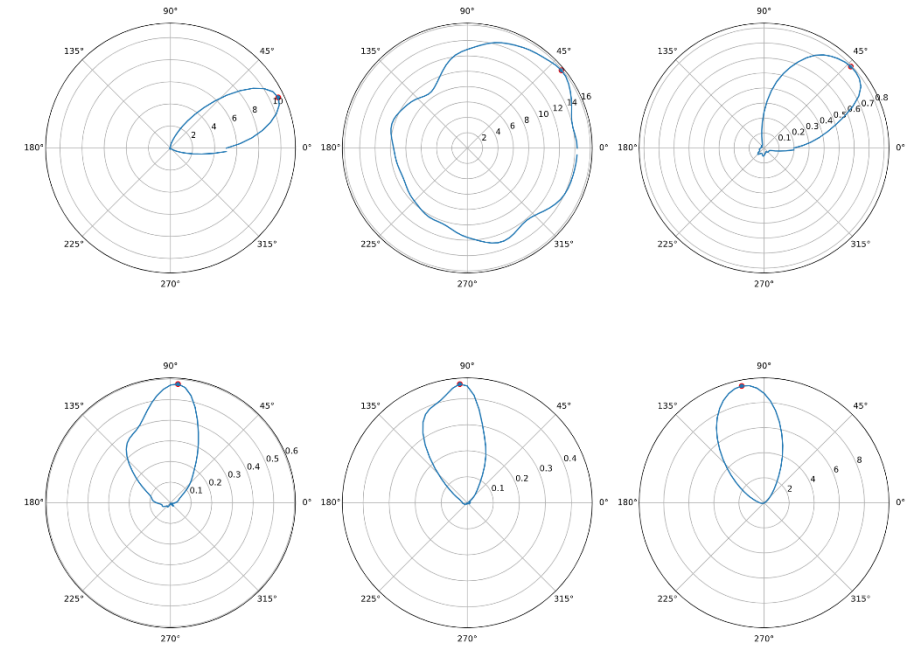
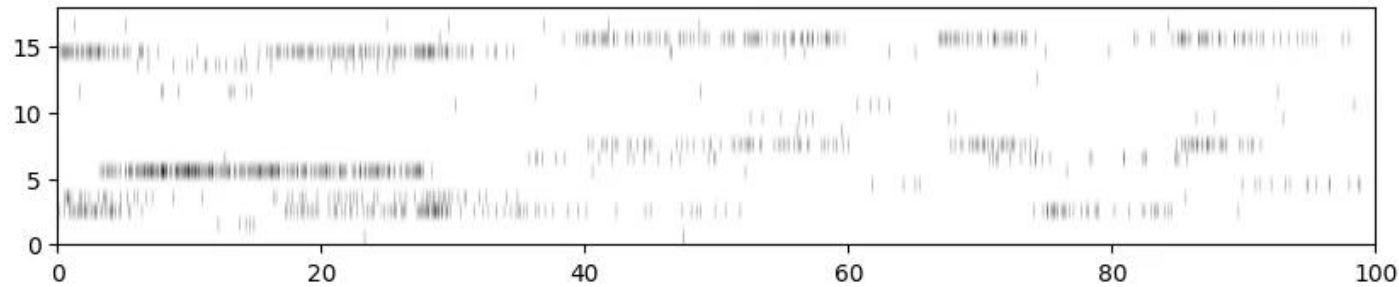
$$n_\xi \sim \mathcal{N}(0, I)$$

$$\text{spike}_t = I_t > \text{threshold}$$

$$s_{t+\Delta t} = s_t + \text{spike}_t - s_t/\tau dt$$

Dataset

Mouse dataset

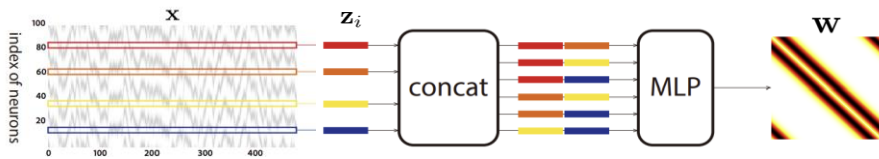


- Selected the top 5 sessions in which each neuron's preferred head direction was uniformly distributed.
- Calculated the preferred head direction of each neuron and removed cells that were difficult to classify as head direction cells

Model

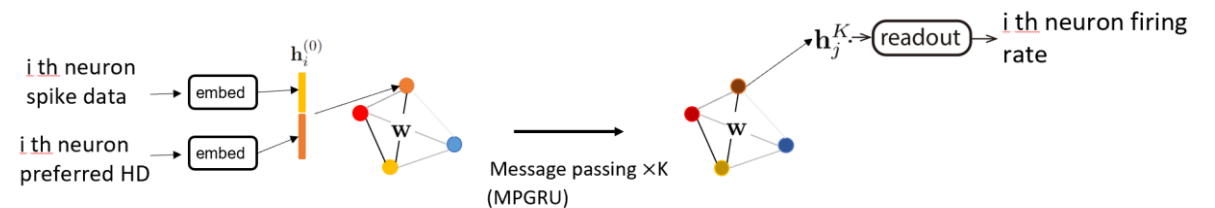
Weight inference module

$$\begin{aligned} \mathbf{h}_i &= f_x(x_i) \\ \mathbf{z}_i &= f_h(\text{vec}(\mathbf{h}_i)) \\ \mathbf{w}_{ij} &= f_z(\mathbf{z}_i \| \mathbf{z}_j) \end{aligned}$$



Spike prediction module

$$\begin{aligned} \mathbf{h}_{x,i}^{(0)} &= f_x(\mathbf{x}_{i,t-L+1:t}) \\ \mathbf{h}_{\theta,i}^{(0)} &= f_{\theta}\left(\theta_t - \frac{2\pi}{N}i - b\right) \\ \mathbf{h}_i^{(0)} &= \begin{bmatrix} \mathbf{h}_{x,i}^{(0)} \\ \mathbf{h}_{\theta,i}^{(0)} \end{bmatrix} \\ \mathbf{m}_{ij}^{(r)} &= \psi\left(\mathbf{h}_i^{(r)} - \mathbf{h}_j^{(r)}\right) \\ \mathbf{h}_i^{(r+1)} &= \phi\left(\mathbf{h}_i^{(r)}, [\mathbf{h}_i^{(0)}, \sum_{j \neq i} w_{ij} \cdot \mathbf{m}_{ij}^{(r)}]\right) \\ \log(\lambda_t) &= f_o\left(\mathbf{h}_i^{(r+1)}\right) \end{aligned}$$



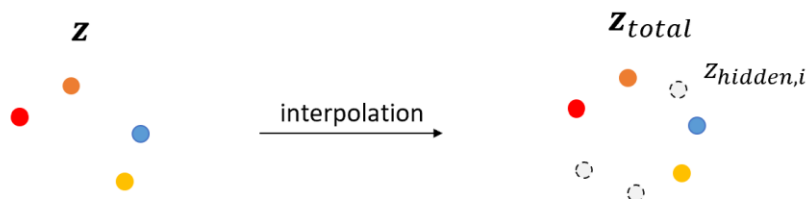
Model

Weight inference module

$$\mathbf{z}_{o,i} = f_h(\text{vec}(\mathbf{h}_i))$$

$$\mathbf{z}_{h,i} = \frac{(\theta_{o,j+1}^* - \theta_{h,i}^*)\mathbf{z}_{o,j} + (\theta_{h,i}^* - \theta_{o,j}^*)\mathbf{z}_{o,j+1}}{\theta_{o,j+1}^* - \theta_{o,j}^*}$$

$$\mathbf{z}_i = [\mathbf{z}_{o,i} || \mathbf{z}_{h,i}]$$



Spike prediction module

$$H_x^t = [f_x(X^{t-L+1:t}) || \text{zeros}]$$

$$H_\theta^t = f_\theta\left(\theta_t - \frac{2\pi}{N}x - b\right)$$

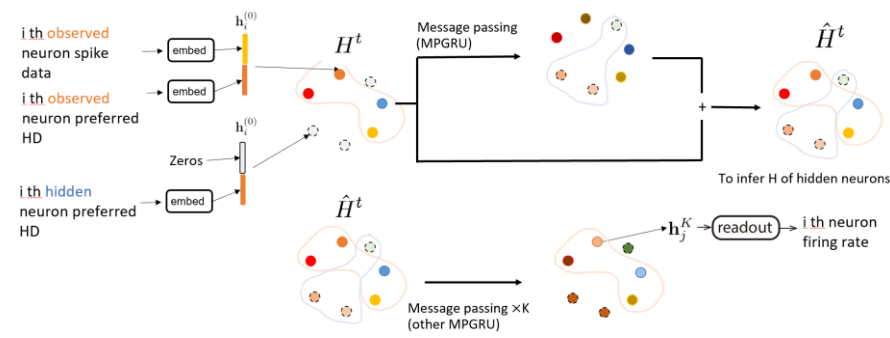
$$H^t = \begin{bmatrix} H_x^t \\ H_\theta^t \end{bmatrix}$$

$$A^t = \text{MPGRU}(H^t)$$

$$\hat{H}^t = m_{ob} \odot H^t + m_{hd} \odot A^t$$

$$\hat{P}^t = \text{MPGRU}(\hat{H}^t)$$

$$\log(\lambda^t) = f_{out}(m_{ob} \odot \hat{P}^t)$$



Experiments

Dataset

- Mouse Head direction cell (5 sessions)
- Synthetic (8mins/ 480,000ms)
 - Multiple bump w/o external input
 - One bump w/o external input
 - One bump with external input
 - Sampled as real data
- Predict the next 10 time steps based on the past 200 time steps
- 1/10 as a validation set, 1/10 as a test set, 8/10 as a training set

Training

- Training Loss

$$\Theta^*, \mathbf{w} = \arg \min_{\Theta} \sum_{i=1}^N \sum_{t=1}^L (\lambda_i^t - x_i^t \log \lambda_i^t)$$

- Prediction accuracy

$$\mathcal{L}_i^{\text{bps}} = \frac{\sum_{t=1}^L [(x_i^t \log \lambda_i^t - \lambda_i^t) - (x_i^t \log \bar{\lambda}_i - \bar{\lambda}_i)]}{\sum_{t=1}^L x_i^t}$$

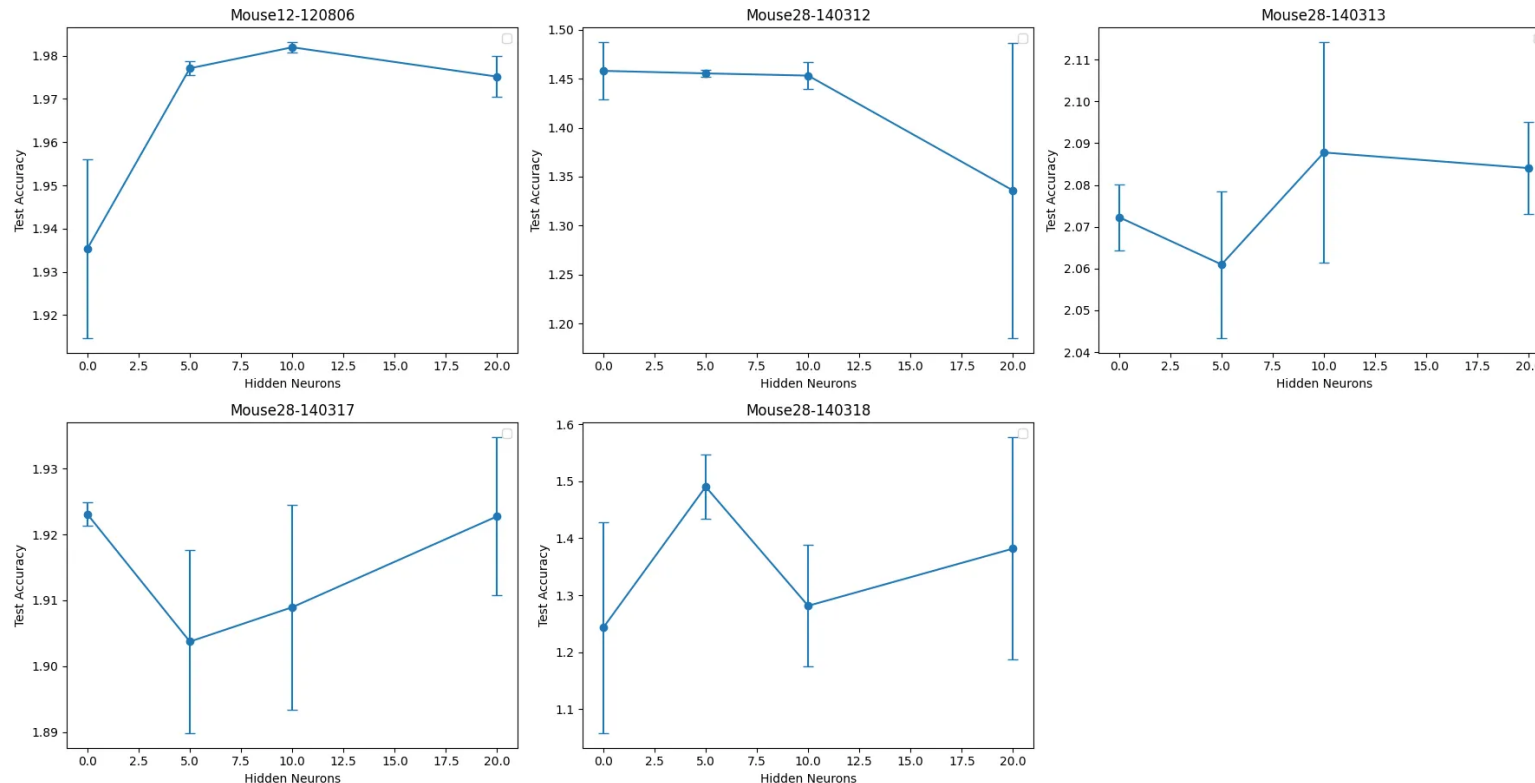
$$\mathcal{L}^{\text{bps}} = \frac{1}{N} \sum_{i=1}^N \mathcal{L}_i^{\text{bps}}$$

Results

Effect of hidden neurons

Synthetic data

- One bump with external input + sampled as real data (17~21 neurons)



Future work

- We can also infer connectivity from cells such as **grid cells**, not just head direction cells.
- We can perform a multivariate time series forecasting task using **hidden neurons** in graph-type data, rather than using neural spike data.

Summary

- We were able to infer the **connectivity** using the spike data from **actual head direction cells** of a rat.
- We were able to improve test accuracy and connectivity inference by assuming **hidden nodes** on GNN.

Reference

- Connectomics: A new paradigm for understanding brain disease, Alex, 2015
- Whole-brain estimates of directed connectivity for human connectomics, Stefan, 2021
- Fly brain breakthrough 'huge leap' to unlock human mind, Pallab Ghosh, 2024
- Neuronal wiring diagram of an adult brain, Sven, 2024
- What Is the Human Connectome Project? Why Should You Care?, Christopher Bergland, 2013
- Neural Relational Inference for Interacting Systems, Kipf, 2018
- Discrete Graph Structure Learning for Forecasting Multiple Time Series, Shang, 2021
- Systematic errors in connectivity inferred from activity in strongly recurrent network, Fiete, 2020
- Graph Neural Networks for Connectivity Inference in Spatially Patterned Neural Responses, Park, 2022